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DIFFUSION COEFFICIENT ON STOCHASTIC CAYLEY TREES*

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Lorentz lattice gases have often been used as models to study diffusion phenomena [4]. In these models, a particle moves ballistically in a d-dimensional regular lattice until it collides with a fixed scatterer. If the particle is moving along the direction j and hits a scatterer of type a, it has a probability W_{aij} of being deflected along the direction i. These scatterers, usually point-like, are placed randomly on the sites of the lattice according to the set of densities ρ_a ($\sum_a \rho_a = \rho$). The statistical quantities of interest are defined as an average over all trajectories in a given quenched configuration of scatterers, followed by an average over all of these configurations. To fix ideas, let us consider the rotator model on a square lattice, so that the particle velocity is a vector taken from the set of four unit vectors connecting every site with its nearest-neighbors. In it, a fraction x_R of the scatterers are stochastic right rotators, a fraction x_L are stochastic left rotators, and a fraction $x_B = 1 - x_R - x_L$ are deterministic backscatterers. When the particle collides with a right (left) rotator, it is deflected to the right (left), transmitted, deflected to the left (right), or reflected with probabilities α_1, α_2, α_3, and $\beta = 1 - \alpha_1 - \alpha_2 - \alpha_3$, respectively. If the collision takes place with a pure backscatterer, the particle is reflected with a probability 1.

These models have usually been studied in the zero density limit, $\rho \to 0$. In this limit, all the trajectories are loopless structures called Cayley trees [1] but, in spite of this simplification, a general analytical solution for the statistical quantities of interest in this problem, such as the diffusion coefficient, remains unknown. The main reason for such a mathematical difficulty is the existence of strong correlation effects caused by the collisions of the moving particle with scatterers visited before. These recollisions are unavoidable (even in the zero density limit) because any reflected particle must collide with a previously visited scatterer as a consequence of the discrete nature of the velocity space. The Boltzmann approximation, which ignores these correlations, becomes very poor for these models and it is necessary to compute the effect of these correlations if better predictions of the statistical quantities are required.

Nevertheless, some particular models have been exactly solved. One of these models is the Cayley tree with a *single type* of scatterers, whose diffusion coefficient was analytically computed by van Beijeren and Ernst [7] by using an exact enumeration of all returning trajectories. Very recently, van Beijeren [8] has also found an exact expression for the diffusion coefficient on the Cayley tree with a mixture of *deterministic* rotators and pure backscatterers (the Cayley-tree version of the Gunn-Ortuño model [5]).

A first attempt to incorporate correlation effects in the expression for the diffusion coefficient was carried out by Ossendrijver, Santos, and Ernst [6] in the so-called repeated ring approximation (RRA). These authors included the repeated ring collisions (trajectories of the form $A - A - A - A$, corresponding to repeated visits of the moving particle to the site A through paths of uncorrelated collisions) by proposing

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a corrected collision operator as follows:

$$\Lambda = -\sum_a \rho_a \{T_a + T_a R T_a + T_a R T_a R T_a + \cdots\} = -\sum_a \frac{\rho_a T_a}{\mathbf{1} - R T_a} , \tag{1}$$

where $T_a = W_a - \mathbf{1}$ and R is the ring operator. The element R_{ij} represents the total return probability with arrival velocity $\mathbf{c}_i$ to a site visited before, when its departure velocity was $\mathbf{c}_j$. By using standard techniques [6] of kinetic theory, the operator R can be related to Λ and the corresponding matrix equation is then solved in a self-consistent way. But the resulting predictions for the diffusion coefficient D are poor, except for models with a mixture of symmetric scatterers (left and right rotators, for example) and without pure backscatterers [1].

We have developed a mean-field theory for Cayley trees which predicts the exact diffusion coefficient in the identical scatterer limit and gives a reasonable estimate for any other model with a mixture of scatterers [2, 3]. More specifically, we propose a mean-field expression for R as

$$R = \mathbf{1} + X + X^2 + \ldots = \frac{X}{\mathbf{1} - X} , \tag{2}$$

where X is the matrix of first return probabilities. Then, the relevant eigenvalues of R are $r_1 = r_3 = -x/(1+x)$, where x is the probability of first return. Substitution of this result into Eq. (1) gives us the eigenvalues λ_1 and λ_3 . The diffusion coefficient is related to these eigenvalues by $D = (1/4\rho)(\lambda_1^{-1} + \lambda_1^{-3})$. To calculate D from this relation we still need an analytical or numerical estimate for the probability of first return, x, since λ_1 and λ_3 depend on it. We have developed a mean-field theory for x [2] and a series of improved numerical renormalization theories [3]. By using the prediction of these theories for x as input in the expression for the diffusion coefficient, we have found that the agreement with the simulation results for several rotator and mirror models is excellent in the range $x_B < 0.4$, although the agreement worsens in the percolation region [3]. Nevertheless, our approximation predicts the diffusive percolation threshold $x_B^c = 2/3$, which agrees with the simulations. In contrast, the repeated ring approximation always predicts a too small threshold $x_B^c = 1/3$ for any model with pure backscatterers in the square lattice.

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